Low energy excitations in fermionic spin glasses: a quantum–dynamical image of Parisi symmetry breaking

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We report large effects of Parisi replica permutation symmetry breaking (RPSB) on elementary excitations of fermionic systems with frustrated magnetic interactions. The electronic density of states is obtained exactly in the zero temperature limit for $(K = 1)$–step RPSB together with exact relations for arbitrary breaking K, which lead to a new fermionic and dynamical Parisi solution at $K = \infty$. The Ward identity for charge conservation indicates RPSB–effects on the conductivity in metallic quantum spin glasses. This implies that RPSB is essential for any fermionic system showing spin glass sections within its phase diagram. An astonishing similarity with a neural network problem is also observed.

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We present the first solution to the question whether and in which way Parisi replica permutation symmetry breaking (RPSB) and the related nonconstant part of the Parisi spin glass order parameter function $q(x)$ [1–3] are displayed in the low temperature many body theory of fermionic systems with frustrated Ising–interactions, emphasizing the $T = 0$–limit in particular. The Parisi function $q(x)$, defined on the interval $0 \leq x \leq 1$ is known as the apparently exact solution of the infinite range classical spin glass. The x–dependence is known to be comparable with a nontrivial time–dependence, induced by Glauber dynamics [2], of the spin autocorrelation function $< \sigma(\tau_x)\sigma(0) >$ (small x corresponding to large times). As shown by Parisi the function $q(x)$ assumes a plateau value within $x_1 \leq x \leq 1$ and differs from this sofar conventional single order parameter picture only within $0 \leq x \leq x_1 = O(T)$, where it decreases towards zero at $x = 0$ in the absence of a magnetic field. The RPSB–effect appears to disappear with $T \to 0$. Nevertheless we find and report here a large $O(T^0)$–effect to persist in many important physical quantities of the fermionic Ising spin glass, which is a minimal quantum generalization of the classical Sherrington Kirkpatrick model. This includes replica–diagonal fermion Green's function and fermion density of states, where at any step K of RPSB the set of different order parameters is seen to determine the quantum–dynamical behaviour of the fermion propagator and of vertex functions. These effects are complementary to and not in contradiction with recent replica–symmetric descriptions of $T = 0$ quantum spin glass transitions [4]. Parisi–RPSB [1] is seen to decide the qualitative and quantitative features of the low energy excitation spectrum. While results are presented for an insulating model, the effect appears to be rather model–independent and should hence be felt in transport properties of models with additional hopping hamiltonian for example.

The presence of spin glass phases within phase diagrams of interacting many–fermion systems such as High$T_c$superconductors, heavy fermion systems, and semiconductors are nowadays recognized with increasing attention [5–7]. Many of their characteristic properties cannot be answered by considering these phases as isolated magnetic phenomena, which means that their common origin, their coexistence and competition with charge–related phenomena, and even far–reaching links into other fields of physics must be understood in terms of fermionic rather than spin space models. The relationship between conductivity behaviour and magnetism, mainly antiferromagnetism up to now, has acquired a prominent place in the conscience of theorists and experimentalists, due to the remarkable progress in the field of strongly correlated fermion systems during recent years [8,9].

In this Letter we wish to provide results which evidence the fact that fermionic spin glasses also link closely glassy magnetic order and transport behaviour; further similarities between Hubbard model and the fermionic spin glass have been traced back to the particular role of the Onsager–Brout–Thomas reaction field [2,8] for all these systems, as can be observed by comparing Hubbard–CPA– [8] with fermionic TAP–equations [7].

Spin– and charge–excitation spectra of fermionic spin glasses must be evaluated in order to construct a meaningful many body theory. This Letter focusses on the effect of Parisi replica permutation symmetry breaking (RPSB) on the single fermion density of states (DoS), hence on the fermionic Green's function, and, by virtue of the Ward identity for charge conservation, also on vertex functions, thus on the entire ensemble of quantities that provide the basis of many body theories for fermionic systems with frustrated interactions.

It is known that replica–diagonal quantities like the linear equilibrium susceptibility χ feel Parisi symmetry breaking even at $T = 0$ [1–3] despite the fact that the nontrivial part of the Parisi function only lives on an interval of width T.

The susceptibility had been analysed by Parisi for the standard SK–model. He found a rapid convergence towards

the exact result as the number of order parameters increased, this number being equal to $K+1$ in the SK– and equal to $K+2$ in fermionic models. While the low temperature regime of the SK–model had not been of particular interest from the point of view of phase transition theory, it becomes highly important for fermionic spin glasses, since the $T=0$–theory of excitation spectra plays a crucial role and, for the additional reason that some models exhibit quantum phase transitions along the $T=0$–axis. Parisi nevertheless analysed the low T regime [1] of the classical SK–model finding that K–step RPSB on one hand provided increasingly good approximations but failed to completely remove the negative entropy and the instability problem at low enough temperatures unless $K\to\infty$.

In this Letter the effect of one step RPSB ($K=1$) on the density of states is presented in detail, followed then by an analytical relation valid for all K, which allows to determine the type of excitation spectrum present in the full Parisi solution for the fermionic Ising spin glass. Despite the fact that the regime of deviation from a replica–symmetric spin glass order parameter is only of $O(T)$, we find that it has a large $O(T^0)$–effect on the fermion density of states, the one–particle–, and many–particle Greens functions at $T=0$. This density of states is derived as usual from the imaginary–time (disorder–averaged) fermion Green's function $[-<T_\tau[a(\tau)a^\dagger(0)]>]_{av}$, which is one of the decisive quantum–dynamical elements of any many body theory of fermionic spin glasses. This illustrates that, unlike the usual picture of a Parisi solution being just a static order parameter function, the fermionic picture must include the qualitative extension to dynamical quantities. Those become drastically altered by the nontrivial part of the Parisi solution which is otherwise invisible at $T=0$, hence providing a *quantum–dynamical image of RPSB.* We first consider a generalized Parisi solution of the infinite–range fermionic Ising spin glass model. Its grand canonical Hamiltonian

$$\mathcal{H}=-\sum_{ij}J_{ij}\hat\sigma_i\hat\sigma_j-H\sum_i\hat\sigma_i-\mu\sum_i(\hat n_{i\uparrow}+\hat n_{i\downarrow}),\quad \hat\sigma_i\equiv\hat n_{i\uparrow}-\hat n_{i\downarrow},\quad \hat n_{i\sigma}\equiv a^\dagger_{i\sigma}a_{i\sigma}, \tag{1}$$

with fermion operators $a, a^\dagger$ and represents a Fock space extension of the SK–model. The magnetic couplings J_{ij} of this insulating model are independent gaussian variables with zero mean value. The chemical potential controls the occupation of magnetic and nonmagnetic states, where the latter ones reduce the freezing temperature, and leads to remarkable effects in the tricritical phase diagram [11]. We restrict our discussion to half–filling. The fermion Green's function can be derived as $\mathcal{G}=\frac{\delta}{\delta\bar\eta}\frac{\delta}{\delta\eta}ln\Xi$ from the generating functional (generalization from $K=1$–step RPSB, given here for the sake of simplicity, to arbitrary K is standard)

$$\Xi_n(\eta,\bar\eta)=e^{-\frac{N}{4}\beta^2J^2TrQ^2_{Parisi}}\prod\int_{-\infty}^{\infty}\frac{dz_\gamma^{(\alpha_\gamma)}}{\sqrt{2\pi}}e^{-\frac{[z_\gamma^{(\alpha_\gamma)}]^2}{2}}\prod\int d\bar\psi d\psi Exp[\sum_{\alpha_1=1}^{n/m}\sum_{a=(\alpha_1-1)m+1}^{\alpha_1 m}$$
$$\sum_{i,\sigma,\epsilon_l}(\bar\psi^{a,l}_{i,\sigma}[\mathcal{G}_0^{-1}(\epsilon_l)+\sigma\tilde H(\{z_\gamma^{(\alpha_\gamma)}\})]\psi^{a,l}_{i,\sigma}+\eta^{a,l}_{i,\sigma}\bar\psi^{a,l}_{i,\sigma}-\bar\eta^{a,l}_{i,\sigma}\psi^{a,l}_{i,\sigma})] \tag{2}$$

with a bare propagator $\mathcal{G}_0(\epsilon_l)=(i\epsilon_l+\mu)^{-1}$ and a magnetic field H included in the effective field $\tilde H(\{z_\gamma^{(\alpha_\gamma)}\})=H+J\sum_\gamma\sqrt{q_\gamma-q_{\gamma+1}}z_\gamma^{(\alpha_\gamma)}$, where $q_0\equiv\tilde q$, $q_{K+1}=0$. Fermionic fields are denoted $\psi,\bar\psi$, and $\eta,\bar\eta$. Spin (decoupling)–fields z_γ, carrying a Parisi block index, explore the random magnetic order. The Parisi matrix Q_{Parisi} has the wellknown form [1] apart from the nonvanishing diagonal elements $\tilde q$; their presence is required by the fact that $(\hat\sigma^z)^2=(\hat n_\uparrow-\hat n_\downarrow)^2\neq 1$. The structure of the Parisi–matrix is of course responsible for the rather complicated form of the Lagrangian; despite this complication the fermion fields can be eliminated in the standard way, which leads to the selfconsistent equations given below.

It is known since Parisi's work [1] that an analytical low temperature expansion is hard to obtain even for the standard SK–model and its smaller set of selfconsistent parameters. First insight is gained by the one–step RPSB ($K=1$). The standard three parameter set of the SK–model for $K=1$, order parameters q_1 and q_2, and $m\equiv m_1\sim T$, is enlarged in the fermionic space by $\tilde q-q_1\sim T$, where $\tilde q:=[<\sigma(\tau)\sigma(\tau')>]_{av}$ represents a spin correlation, which remains static unless a fermion hopping mechanism or other noncommuting parts are included in the Hamiltonian. For the fermionic Ising spin glass the $(K=1)$–DoS reads

$$\rho_\sigma(E)=\frac{ch(\beta\mu)+ch(\beta E)}{\sqrt{2\pi(\tilde q-q_1)}J}\frac{e^{-\frac12\beta^2J^2(\tilde q-q_1)}}{\sqrt{2\pi q_2}}\int_{-\infty}^{\infty}dv_2e^{-\frac{v_2^2}{2q_2}}\frac{\int_{-\infty}^{\infty}dv_1e^{-\frac{(v_1-v_2)^2}{2(q_1-q_2)}-\frac{(v_1+H+\sigma E)^2}{2(\tilde q-q_1)}}\mathcal{C}^{m-1}}{\int_{-\infty}^{\infty}dv_1e^{-\frac{(v_1-v_2)^2}{2(q_1-q_2)}}\mathcal{C}^m} \tag{3}$$

with $\mathcal{C}=cosh(\beta\tilde H)+\zeta$, where $\zeta=cosh(\beta\mu)exp(-\frac12\beta^2(\tilde q-q_1))$ reveals the competition between the particle "pressure" exerted by the chemical potential μ and the single–valley susceptibility $\bar\chi=\beta(\tilde q-q_1)$ leading to a crossover at $|\mu|=\frac12\bar\chi$ in the $T\to0$–limit. The ζ–term is a fermionic feature, absent from the standard SK–model. It is closely related to the fermion filling; this filling factor behaves discontinuously on the $T=0$–axis [11]. For $T=0$ we obtain exactly

$$\rho_\sigma(E) = \frac{e^{-\frac{1}{2}a^2(H)(1-q_2) - \frac{\Delta_E^2}{1-q_2} + a(H)\Delta_E - \frac{H^2}{2q_2}}}{\pi\sqrt{1-q_2(H)}}\Theta(|E|-\bar{\chi})\int_{-\infty}^{\infty} dz \frac{e^{-\frac{1}{2}\frac{z^2}{1-q_2} - (\frac{\sqrt{q_2}}{1-q_2}\frac{\sigma E}{|E|}\Delta_E - \frac{H}{\sqrt{q_2}})z}}{d(z)+d(-z)}, \tag{4}$$

$$d(z) \equiv e^{a(H)\sqrt{q_2}z}\left[1 + Erf(\frac{a(H)(1-q_2)+\sqrt{q_2}z}{\sqrt{2(1-q_2)}})\right], \quad \Delta_E \equiv |E| - \bar{\chi}, \tag{5}$$

and $a(H) \equiv m'(T=0)$. The replica–symmetric solution displays a magnetic hardgap of width $2E_g(H)$ in the DoS and the system remains half–filled at $T=0$ within the finite interval given by $|\mu| < \frac{1}{2}E_g(H)$. For higher values of the chemical potential, hence smaller spin density, phase separation occurs together with a discontinuous transition into a full or an empty system [11]. A stable homogeneous saddle–point solution could only be found for the half–filled case. Thus the following analysis is restricted to this interval of chemical potentials. Its width is determined selfconsistently and seen to decrease to zero as $K \to 0$. The selfconsistent equations for $\tilde{q}, q_1, q_2$ and the Parisi parameter m [1] simplify in the $T=0$–limit becoming

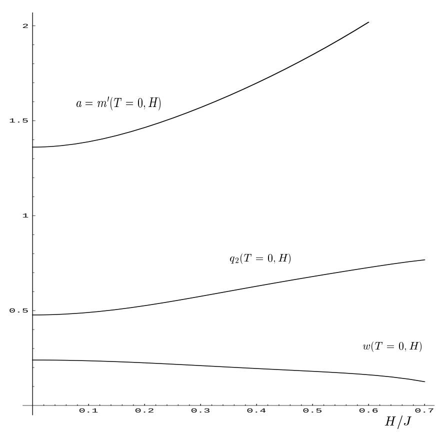
$$\tilde{q} = q_1 = 1, \;\; lim_{T\to 0}\frac{\tilde{q}-q_1}{T} = \bar{\chi}, \;\; q_2 = \int_{-\infty}^{\infty}\frac{dz}{\sqrt{2\pi}}e^{-\frac{(z-H/\sqrt{q_2})^2}{2}}\left[\frac{d(z)-d(-z)}{d(z)+d(-z)}\right]^2 \tag{6}$$

$$\begin{aligned} 0 = 1 - q_2^2 - \frac{4}{a}\int_{-\infty}^{\infty}\frac{dz}{\sqrt{2\pi}}\, e^{-\frac{(H/\sqrt{q_2}-z)^2}{2}}\{-\frac{1}{a}\, ln[\frac{1}{2}e^{\frac{1}{2}a^2 t}(d(z)+d(-z))] \\ +[(at+\sqrt{q_2}\, z)d(z) + (at-\sqrt{q_2}\, z)d(-z) + \sqrt{8t/\pi}\, e^{-\frac{1}{2}a^2 t - \frac{1}{2}q_2 z^2/t}]/[d(z)+d(-z)]\} \end{aligned} \tag{7}$$

where $t \equiv q_1 - q_2$. For zero magnetic field one finds $q_2 = 0.476875, a = lim_{T\to 0}m'(T=0) = 1.36104$, and $\bar{\chi} = lim_{T\to 0}(\tilde{q}-q_1)/T = .239449$. The H–dependent solutions shown in fig.1 are obtained numerically and then used in evaluating eq.(4) for the density of states. $T=0$–results are shown in figs.2 and 3, while the result at finite low temperature of fig.4 illustrates the presence of plateaus of constant slope, each corresponding to Parisi order parameter separations (here: $\tilde{q}-q_1$ and q_1-q_2). The number of these plateaus of constant slope increases with the order K of Parisi–RPSB. Hence, the time–dependence of the Green's function should characteristically depend on the order parameter separations $q_k - q_{k-1}$. If we compare with the replica–symmetric result a reduction of the gapwidth is observed. Analytically one finds a gapwidth

$$E_g(H) = \bar{\chi} = lim_{T\to 0}\beta(\tilde{q}-q_1) \tag{8}$$

which turns into $lim_{T\to 0}(\beta(\tilde{q}-q(1)))$ in terms of the Parisi function at $K=\infty$. Only at zero RPSB this susceptibility coincides with the equilibrium χ. In fact for 1–step RPSB the fermionic Ising spin glass approaches $\chi = \beta(\tilde{q}-q_1) + \beta m(q_1-q_2) \to .95$, the same numerical value as the one for the SK–model.



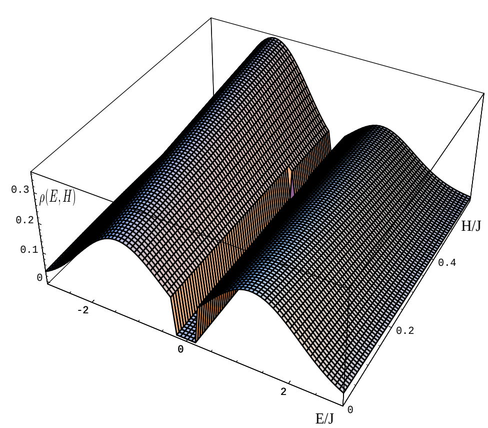
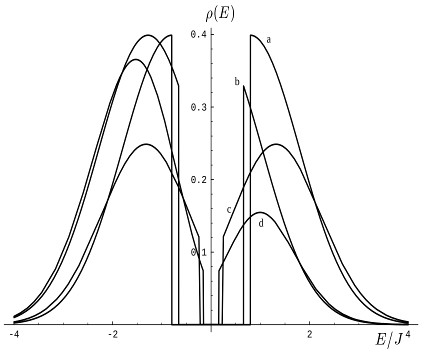


FIG. 1. Field dependence of dm/dT (top), of the order parameter q_2, and of gapwidth parameter w (bottom) for 1RPSB and zero temperature.

FIG. 2. density of states at $T=0$ as a function of energy and magnetic field for 1–step RPSB



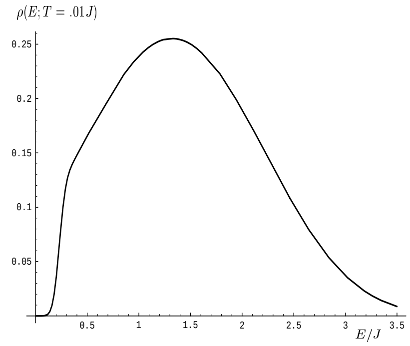


FIG. 3. Effect of one step replica symmetry breaking on the fermionic density of states (DoS) for magnetic fields $H = 0$ (curve c: 1RPSB, a: 0RPSB) and $H/J = 0.6$ (d: 1RPSB, b: 0RPSB)

FIG. 4. Low but finite temperature ($T = .01J$) form of the zero field DoS in 1–step RPSB.

While the 1–step RPSB provides already a much better approximation than 0–RPSB it is still unstable towards higher RPSB. We have therefore extended given equations to arbitrary K. Apart from the K-invariant relation $E_g(H) = \bar{\chi}$ we find a second invariant with respect to K–th RPSB, including $K = \infty$, which is given by

$$lim_{|E|\downarrow E_g(H)} \rho_\sigma(E) = \frac{1}{2}\bar{\chi} = \frac{1}{2}E_g(H) \tag{9}$$

The invariant ratio 1/2 is seen analytically by comparing the formulae for the gapwidth and for $\rho(|E| = E_g + 0)$ (both generalized to arbitrary K) in the $T \to 0$–limit. For each given K, (half) the gapwidth equals the fermionic nonequilibrium susceptibility $\bar{\chi}$, which turns into $\bar{\chi} = \beta(\tilde{q} - q(1))$ differing only by exponentially small terms from the SK–model result $\bar{\chi} = \beta(1 - q(1)) \sim T$ [2], where $q(1)$ denotes the Parisi function $q(x)$ at $x = 1$. Consequently the DoS–hardgaps at finite K terminate in a softgap for $K \to \infty$. Note that we did not have to evaluate the $T = 0$–Parisi function $q(x)$ in order to reach this conclusion. Assuming that the relation between gapwidth and $\bar{\chi}$ remains valid (at least in good approximation) for short–range models, fluctuation effects should harden the gap. This requires further analysis.

A quantity of particular interest in many–body theories is the Ward identity for charge conservation. It shows that Parisi symmetry breaking, as observed in the density of states, exists also in vertex functions. The Ward identity for the insulating model can be viewed as one of a metallic spin glass at momentum transfer $\underline{k} = 0$, ie $i\omega\, \Lambda_n(\underline{k} = 0, \epsilon + \omega, \epsilon) = \mathcal{G}(\epsilon + \omega) - \mathcal{G}(\epsilon)$ (fermion momenta suppressed). Λ_n is the Fourier transformed three point function $< T_\tau[a_i^\dagger(\tau) a_{i'}(\tau') \hat{n}_j(0)] >$ in terms of the fermion operators. Thus the density–part Λ_n in the Ward identity (a current–part $\Lambda_{\underline{j}}$ emerges for itinerant models and $\underline{k} \neq 0$) obeys

$$lim_{\omega\to 0}\, \omega\, lim_{\underline{k}\to 0} \Lambda_n^{AR}(\underline{k}, \epsilon + \omega, \epsilon) = 2\pi i\, \rho(\epsilon, \{q_r - q_{r-1}\}) \tag{10}$$

and thus shows that the Parisi form of the DoS, depending on all $q_r - q_{r-1}$ or on $q(x)$ for $K = \infty$, also enters the vertex function. This will also occur in metallic spin glases, whence diffusive modes and conductivity are expected to depend on Parisi symmetry breaking. While we have proved the existence of a spin–glass hardgap at any finite $K > 0$ with

$$\delta\rho(E) \sim |E - w(H)| \quad , [|E| \geq \bar{\chi}, K < \infty]; \qquad \rho(E) \sim |E|^x, [K = \infty] \tag{11}$$

the pseudogap solution at $K = \infty$ has a scaling exponent x, which could eventually become different from one and remains to be determined. This pseudogap together with x=1 would be slightly reminiscent of the exponent found for a superconducting glass unitary nonlinear sigma model [10]. We remark that the pseudogap–solution given for the fermionic spin glass model refers precisely to $\mu = 0$ whereas the hardgap–solutions at finite K happened to be stable within finite intervals $|\mu| \leq \bar{\chi}/2$ corresponding to half–filling only at $T = 0$. The regime beyond half–filling, identified as the domain of phase separation in the replica–symmetric solution [11], requires further analysis at $T = 0$ as well as several metallic–, Kondo–type–, superconducting–, and other model extensions. The new method of Fourier Transformations in replica space [12] is hoped to facilitate further insight into the difficult $K = \infty$–solutions.

We note that an overlap distribution function for data clustering shown in [13] and interpreted as a pseudo $T = 0$–problem in a classical spin analogy, revealed, apart from the ratio discussed in Eq.(9), a remarkable similarity with the $(H = 0)$–density of states. It appears interesting to explore pseudo–$(T = 0)$ neural network problems [14] as

potential classical partners of fermionic spin glasses.
Summarizing our results we proved i) replica permutation symmetry breaking to be most important in the $T = 0$ quantum field theory of the fermionic spin glass, ii) that low energy excitations are determined by RPSB and hence the long–time quantum–dynamical behaviour of the fermion Green's function carries RPSB–fingerprints, which iii) affects higher order correlations by means of charge conservation too.
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